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A comparative study of the harmonic balance method and the orthogonal collocation method on stiff non linear systems

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Abstract

The high-order purely frequency-based Harmonic Balance Method (HBM) presented by Cochelin and Vergez [1] and extended by Karkar et al. [2] now allows to follow the periodic solutions of regularized non-smooth systems (stiff systems). This paper compares its convergence property to a reference method in applied mathematics: orthogonal collocation with piecewise polynomials. A first test is conducted on a nonlinear smooth 2 degree-of-freedom spring mass system, showing better convergence of the HBM. The second test is conducted on a one degree-of-freedom vibro-impact system with a very stiff regularization of the impact law. The HBM continuation of the nonlinear mode was found to be very robust, even with a very large number of harmonics. Surprisingly, the convergence was again found to be better than the one of the collocation method for this vibro-impact system.

Keywords: nonlinear dynamical systems, periodic solutions, asymptotic numerical method, harmonic balance, orthogonal collocation

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1. Introduction

The literature is crudely lacking comparative studies between purely time-based and purely frequency-based numerical methods for computing periodic solutions of nonlinear dynamical systems. This is especially true regarding the behavior of numerical methods when addressing stiff mechanical systems like impacting oscillators (vibro-impact system). This paper aims at comparing two such methods, in a general framework where one wishes to compute families, or branches, of periodic solutions of such systems using a numerical continuation algorithm. This is an important issue in many scientific fields and engineering applications.

In literature, various numerical methods have been proposed to directly compute such periodic solutions [3–6] without resorting to numerical time integration techniques, which provide stable periodic solutions only as a limit set and can be very time-consuming, especially for stiff systems. These direct numerical methods are generally classified into two main categories referred to as the frequency domain approach and the time domain approach.

The emblematic method for the frequency domain approach is the so-called harmonic balance method (HBM) which relies on the representation of the periodic orbit by a truncated Fourier series for the unknown state variables. The HBM substitutes the series into the nonlinear governing equation, collecting terms with the same harmonic number and dropping terms with harmonic numbers not in the Fourier series. This leads to solving an algebraic system for the Fourier coefficients which balances harmonics. HBM is better presented as a weighted residual method: it is a Galerkin method with Fourier basis and Fourier test functions, and for which convergence has been established for instance by Urabe [7]. Note that some authors describe the HBM as unpractical or cumbersome, as it implies analytical derivation

28 of the relations between Fourier coefficients involved in the nonlinear terms.
 29 However, previous works have shown that: first, most nonlinearities can be
 30 recast as quadratic polynomials using additional variables; and second, in
 31 the quadratic case it is very easy to automate this analytical work (see [2]).
 32 Many variations of the basic HBM exist, such as the Alternating Frequency
 33 Time-HBM [8], the Multi-HBM [9], the Incremental HBM [10], the Adaptive
 34 HBM [11]. Some of these variations improve usability, performance, or ro-
 35 bustness. Some adapt to situations such as non-smooth systems [12] or delay
 36 systems for example.

37 Two emblematic methods for the time domain approach are the shooting
 38 method [4, 5] (not considered here, as it does use time integration) and
 39 the global finding of periodic orbits using a boundary value approach [6].
 40 The orthogonal collocation with piecewise polynomials (later referred to as
 41 collocation) belongs to the second one: the periodic orbit is divided into mesh
 42 intervals, the unknown state variables are represented by polynomials on each
 43 interval and the governing equations are collocated at Gauss points. This
 44 collocation method may also be seen as a weighted residual method (in this
 45 case, a Petrov-Galerkin method) with piecewise polynomial basis and Dirac
 46 test functions, and many variations exist. To end, it is worth noting note that
 47 a third category could have been introduced for trigonometric collocation
 48 methods [13], or similarly the High-Dimensional HBM [14] which, despite
 49 the name, is more a collocation method than an HBM as shown by [15].
 50 Methods belonging to the latest category are once more weighted residual
 51 methods, but with Fourier basis and Dirac test function.

52 Today, HBM is very popular in electrical engineering (electronic circuit)
 53 and in mechanical engineering (structural dynamics, rotor dynamics) while
 54 the collocation method is very popular for biological systems, population sys-

55 tems, chemical reactions analysis and more generally for applied mathematics
56 (the collocation method is for instance implemented in the AUTO software
57 [16], as well as in the MATCONT package [17], a MATLAB [18] toolbox).
58 So, it seems that the choice between the frequency domain approach and
59 the time domain approach is not only a question of performance and ease of
60 implementation, but also a question of experience inside a scientific field. As
61 stated earlier, the literature lacks comparisons between these two categories
62 of methods: typical papers describe a numerical method and demonstrate
63 its performance on selected representative examples, but comparisons are
64 seldom performed.

65 The present study compares the high-order purely frequency HBM pre-
66 sented in [1] and extended in [2], with the piecewise polynomial collocation
67 method. For this, a still challenging mechanical problem is chosen: periodic
68 solutions continuation of a regularized vibro-impact system, that is, nonlin-
69 ear mode calculations of a non-smooth system. The comparison is carried
70 out using the asymptotic numerical method (ANM) for the continuation and
71 each of the aforementioned methods for the discretization. Because many
72 variations exist for each category of methods, a few conditions have to be
73 fixed for the comparison. Hereafter, focus is brought to the accuracy of the
74 solution versus the number of unknowns in the algebraic system. Second, the
75 comparison is limited to small size dynamical systems. Third, no adaptive
76 mesh is used for the collocation and no harmonic selection is used for the
77 HBM. Within this framework, and despite the common wisdom that would
78 advise against using the HBM for systems with stiff nonlinearities, the HBM
79 achieves a better convergence rate than the collocation, even for very stiff
80 problem.

81 The paper is organized as follows: in section 2, the harmonic balance
 82 method and the orthogonal collocation with piecewise polynomials method
 83 are reviewed, and their theoretical convergence rates are recalled. In section
 84 3, their convergences are compared on a toy-model composed of a slightly
 85 nonlinear, one-mass, two-spring plane system (representative of shells under
 86 large strain), as well as their efficiency for calculating periodic orbit families,
 87 when coupled with the ANM continuation technique. Then, in section 4, the
 88 same methodology is used to compare both approaches on a highly nonlin-
 89 ear system: an impacting oscillator with exponential restoration force. The
 90 conclusions of this comparative study are outlined in the last section.

91 2. Discretization methods for periodic orbits

In this section, the two methods that are used here for solving the periodic boundary-value problem that consists in finding a periodic solution of a given autonomous, nonlinear dynamical system are briefly reviewed. The problem is to find $\mathbf{Y} : \mathbb{R} \rightarrow \mathbb{R}^n$ and its associated period $T \in \mathbb{R}_+$ such that $\forall t \in \mathbb{R}$,

$$\mathbf{Y}'(t) = f(\mathbf{Y}(t)) \quad (1)$$

$$\mathbf{Y}(t) = \mathbf{Y}(t + T) \quad (2)$$

92 where f is a nonlinear application $\mathbb{R}^n \rightarrow \mathbb{R}^n$ and the prime sign denotes the
 93 time derivative.

94 The general principle of a spectral method is to choose a vector-space \mathbb{E}
 95 in which one wishes to approximate the solutions, together with a basis of
 96 this space: the representation functions $\{\phi_i(t)\}$. Then one writes a num-
 97 ber of algebraic equations resulting from the orthogonalization of the residue
 98 $\mathcal{R}(\mathbf{Y}(t)) = \mathbf{Y}'(t) - f(\mathbf{Y}(t))$ to this vector-space, with respect to the corre-
 99 sponding scalar product. This second step is usually carried out by canceling

100 out the projection of the system's ordinary differential equations onto a set
 101 of functions, usually but not necessarily a basis of \mathbb{E} : the test (or weighting)
 102 functions. The reader is referred to Orszag [19] and Karniadakis and Sher-
 103 win [20] for the original works and a recent reformulation on spectral and
 104 pseudo-spectral methods.

105 2.1. The harmonic balance method

106 In the case of the harmonic balance method, the solution of (1-2) is
 107 approximated with a truncated Fourier series:

$$\hat{\mathbf{Y}}(t) = \mathbf{Y}_0 + \sum_{k=1}^H \mathbf{Y}_{2k-1} \cos(k\omega t) + \mathbf{Y}_{2k} \sin(k\omega t)$$

108 the vector-space of the approximation being spanned by the functions:

$$109 \{1, \cos(\omega t), \sin(\omega t), \dots, \cos(H\omega t), \sin(H\omega t)\},$$

110 where $\omega = 2\pi/T$ is the angular frequency of the solution and H the chosen
 111 order of truncation.

112 The *balance* of the harmonics consists in canceling out the projection of
 113 the residue obtained with this truncated series $\mathcal{R}(\hat{\mathbf{Y}}) = \hat{\mathbf{Y}}' - f(\hat{\mathbf{Y}})$ onto
 114 each function of the basis. Thus, the test functions are identical to the
 115 representation functions. The chosen scalar product is defined as:

$$< u, v > = \frac{1}{T} \int_0^T u(t)v(t)dt \quad (3)$$

Thus comes the following $2H + 1$ vector-valued, algebraic equations:

$$\begin{aligned}
& \langle \mathcal{R}(\hat{\mathbf{Y}}), 1 \rangle = 0 \\
& \langle \mathcal{R}(\hat{\mathbf{Y}}), \cos(\omega t) \rangle = 0 \\
& \langle \mathcal{R}(\hat{\mathbf{Y}}), \sin(\omega t) \rangle = 0 \\
& \quad \vdots \\
& \langle \mathcal{R}(\hat{\mathbf{Y}}), \cos(H\omega t) \rangle = 0 \\
& \langle \mathcal{R}(\hat{\mathbf{Y}}), \sin(H\omega t) \rangle = 0
\end{aligned}$$

116 Depending on the form of f and on the number of harmonics H , and
117 using trigonometric identities, an algebraic system is obtained. It consists of
118 $n(2H + 1)$ nonlinear, algebraic equations in the $n(2H + 1)$ unknowns that
119 composes the vector $\{\mathbf{Y}_0^t, \mathbf{Y}_1^t, \mathbf{Y}_2^t, \dots, \mathbf{Y}_{2H-1}^t, \mathbf{Y}_{2H}^t\}^t$ (the notation \cdot^t denoting
120 transposition).

121 In practice, obtaining this system explicitly may be difficult. But in the
122 case where f can be recast as a quadratic polynomial, Cochelin and Vergez
123 [1] showed that the explicit form can be obtained automatically, and for
124 any order of truncation H . The method has been extended to any kind of
125 nonlinearities by Karkar et al. [2].

126 In the case of autonomous systems, to get a well posed problem, one
127 additional equation is needed: when a solution of (1–2) exists, any time-shift
128 of this solution is also a solution. The additional equation is thus known as
129 the *phase equation*, because it is obtained by prescribing the phase of the
130 solution. It is related both to the initial value of the solution, and to the
131 reference used for the time variable. The phase condition may be prescribed
132 several ways, see Doedel [6] and Seydel [5] for details.

In the case of the HBM, *one* coefficient of the Fourier series of *one* com-

ponent of \mathbf{Y} may be set to 0 for the phase equation. This enables to get a well-posed algebraic system $\mathbf{R}(\mathbf{U}) = 0$ of size $n(2H + 1) + 1$ where the unknown vector \mathbf{U} is:

$$\mathbf{U} = [\mathbf{Y}_0^t, \mathbf{Y}_1^t, \dots, \mathbf{Y}_{2H}^t, \omega]^t.$$

133 2.2. Orthogonal collocation at Gauss points with piecewise polynomial

134 The solution of (1–2) is approximated by a continuous, periodic, piecewise
135 polynomial of order p . The chosen collocation scheme is that described in
136 Doedel [6], as used in the AUTO software [16], except for the mesh that is
137 not adaptive in our implementation.

138 First, the period $[0, T]$ is divided into a set of N subintervals $[t_j, t_{j+1}]$,
139 where $h = t_{j+1} - t_j$ is the size of the subintervals, $t_0 = 0$ and $t_N = T$.

140 Then, on each subinterval, the solution is locally sampled in $p + 1$ equidis-
141 tant points, including the subinterval borders:

$$\mathbf{Y}_{j,i} = \mathbf{Y}(t_{j,i}) = \mathbf{Y}(t_j + \frac{i}{p}h), \quad i \in [0..p] \quad (4)$$

142 and interpolated on that interval using the Lagrange polynomials of order
143 p , $\{\ell_{j,i}\}$, based on the $p + 1$ sampling instants $t_{j,i}$:

$$\forall t \in [t_j, t_{j+1}], \quad \hat{\mathbf{Y}}(t) = \sum_{i=0}^p \mathbf{Y}_{j,i} \ell_{j,i}(t) \quad (5)$$

The set of representation functions is obtained by extension of the definition domain of each local Lagrange polynomial $\ell_{j,i}$ to $[0, T]$, setting its value to zero outside of its initial definition domain $[t_j, t_{j+1}]$. Thus, the approximation of the solution is written:

$$\hat{\mathbf{Y}}(t) = \sum_{j=0}^{N-1} \sum_{i=0}^p \mathbf{Y}_{j,i} \ell_{j,i}(t).$$

144 The continuity constraint is imposed by adding the equations $\mathbf{Y}_{j,p} =$
 145 $\mathbf{Y}_{j+1,0}$ for $j = 0..N - 1$, or simply by using the same variable for both vector
 146 of each pair.

147 Here, the test functions are Dirac distributions, centered on each of the p
 148 collocation points of each of the N subintervals: $\delta(t - z_{j,i})$. The p collocation
 149 points of the j -th subinterval $z_{j,i}$ are the Gauss-Legendre points of order p ,
 150 defined as the zeros of the Legendre polynomial of order p on this subinterval.

151 For instance, assuming $p = 3$, the zeros of the third order Legendre poly-
 152 nomial on its standard interval of definition $[-1, 1]$ are located at: $-\sqrt{\frac{3}{5}}, 0, \sqrt{\frac{3}{5}}$.
 153 A translation and a scaling factor is applied in order to get the position of
 154 the $\{z_{j,i}\}_{j=0..N-1, i=1..p}$ relative to the full period $[0, T]$.

155 It is convenient to keep p constant, because if its value were to be modified,
 156 the collocation points positions would need to be computed (at least on
 157 $[-1, 1]$) for every new value. Moreover, preliminary investigations using the
 158 AUTO software with a fixed mesh showed that, for non-smooth or very stiff
 159 systems, increasing the order of polynomials p is more costly and less efficient
 160 than increasing the number of elements N . This needs to be investigated in
 161 future works as the AUTO software restricts the values of p to low integers
 162 ($p \leq 7$).

163 Thus, in what follows, the value $p = 3$ is used. Only the h -refinement
 164 will be considered, that is increasing N .

165 To apply the Petrov-Galerkin method, the residue $\mathcal{R}(\hat{\mathbf{Y}}(t))$ is projected
 166 on every test function and this projection is set to zero. It follows:

$$< \mathcal{R}(\hat{\mathbf{Y}}(t)), \delta(t - z_{j,i}) > = 0 \quad i = 1..p, j = 0..N - 1 \quad (6)$$

167 which reduces to the *collocation* equations:

$$\mathcal{R}(\hat{\mathbf{Y}}(z_{j,i})) = 0 \quad i = 1..p, j = 0..N-1 \quad (7)$$

168 These pNn algebraic equations, together with the periodicity condition
 169 $\mathbf{Y}_{0,0} = \mathbf{Y}_{N-1,p}$ (n equations) and a phase condition (one equation), form an
 170 algebraic system $\mathbf{R}(\mathbf{U}) = 0$ of size $(pN+1)n+1$ where the unknown vector
 171 \mathbf{U} is:

$$\mathbf{U} = [\{\mathbf{Y}_{j,i}^t\}_{\substack{j=0..N-1 \\ i=0..p-1}}, \mathbf{Y}_{N-1,p}^t, T]^t. \quad (8)$$

172 Recalling that $\mathbf{Y}_{j,i} = \hat{\mathbf{Y}}(t_{j,i}) \in \mathbb{R}^n$, the size of the unknown vector \mathbf{U} is
 173 $(pN+1)n+1$, leading to a well posed problem.

174 2.3. Theoretical convergence rates

175 Gottlieb and Orszag [21] proved the convergence for both spectral and
 176 pseudo-spectral methods, under the assumptions of continuity and differen-
 177 tiability of f . The first and most important conclusion they draw is that the
 178 optimal rate of convergence highly depends on the smoothness of the solution
 179 that one tries to approximate, which itself is related to the smoothness of the
 180 function f that describes the system. De Boor and Swartz [22] further im-
 181 proved the p -convergence bound on the collocation method in the particular
 182 case where one uses the Gauss-Legendre points as collocating points.

183 In the case of a smooth solution (suppose, e.g., that f is \mathcal{C}^∞), the HBM
 184 uniform convergence rate is in $\mathcal{O}(c^{-H})$ where $c \in \mathbb{R}_+$ is a constant greater
 185 than 1 and $H \in \mathbb{N}$ is the order of the approximation (the number of har-
 186 monics), whereas the orthogonal collocation at Gauss points has a uniform
 187 convergence rate in $\mathcal{O}(N^{-(p+1)})$ where $N \in \mathbb{N}$ is the number of elements in
 188 one period ($N = T/h$) and $p = 3$ is the order of the polynomial interpolation
 189 chosen for this study, which is also the number of collocation points in each
 190 subinterval.

191 2.4. Continuation

192 The computation of *families* of periodic solutions using numerical contin-
 193 uation assumes the dependence of \mathbf{R} (that is, of f , in the first place) on an
 194 explicit parameter λ . The equation to be solved becomes: $\mathbf{Y}'(t) = f(\mathbf{Y}(t), \lambda)$.
 195 Once discretized, the system reads: $\mathbf{R}(\mathbf{U}, \lambda) = 0$. This nonlinear algebraic
 196 system of N_{tot} equations for $N_{\text{tot}} + 1$ unknowns thus possesses solutions that
 197 form a continuous¹ curve $(\mathbf{U}(\lambda), \lambda)$, known as a solution branch, that is
 198 parametrized (implicitly or explicitly) by the continuation parameter λ .

199 The ANM (“MAN” in French) is a powerful numerical method that allows
 200 for the computation of such branches $\mathbf{U}(\lambda)$ as high-order Taylor series in
 201 λ . The method is implemented in MANlab [23], a toolbox written for the
 202 MATLAB software [18], and both the HBM and the orthogonal collocation
 203 method are implemented on top of the continuation scheme.

204 The following parameters of the ANM have been used in MANlab, and
 205 are kept constant throughout this study, unless stated otherwise:

- 206 • absolute threshold on the norm of the residue for the Newton-Raphson
 207 corrector: $\epsilon_{\text{NR}} = 10^{-9}$ (the residue norm is checked at the end of each
 208 step, and correction is carried out only if necessary),
- 209 • ANM series threshold used for step length estimation: $\epsilon_{\text{ANM}} = 10^{-12}$,
- 210 • ANM series order: $N_{\text{series}} = 20$.

211 The choice of a small correction threshold ensures that the accuracy of a
 212 solution is mainly dependent on the accuracy of the discretization method,
 213 and not on that of the solver of the quadratic problem. Similarly, the choice
 214 of an even smaller ANM threshold ensures that the approximation at the end

¹At least locally, and in the absence of bifurcation.

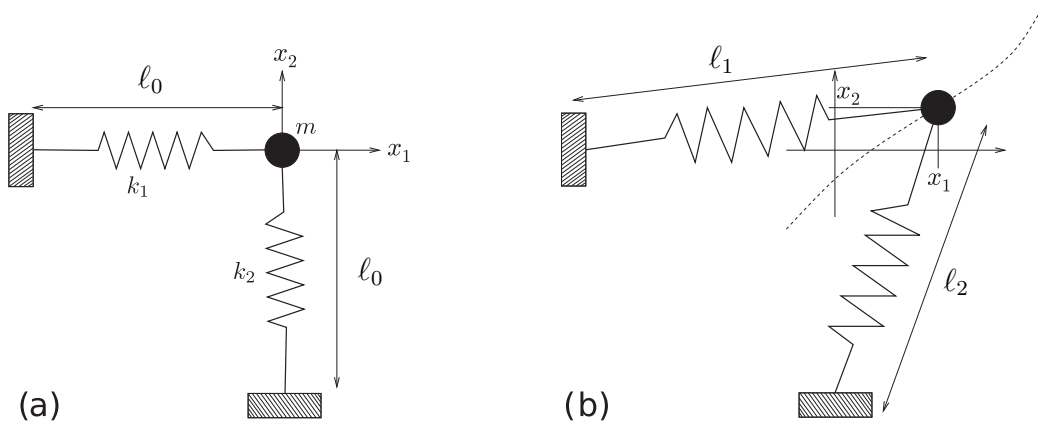


Figure 1: Sketch of the weakly nonlinear system: a mass m attached with two springs of strengths k_1 and k_2 . **(a)** At rest the mass position is $(0, 0)$ and the springs are perpendicular with an identical length ℓ_0 . **(b)** Taken away from its rest position, the mass position is noted (x_1, x_2) and the length of the springs are noted ℓ_1 and ℓ_2 .

215 of each step is accurate enough so that no correction is usually needed at the
 216 beginning of the next step. Finally, the choice of the series order is arbitrary
 217 and mainly influences the step length.

218 3. Comparative study, case 1 : a weakly nonlinear system

219 3.1. A toy model with large displacements and geometrical nonlinearities

220 In this example, a point mass m is constrained by two perpendicular
 221 springs (at rest) of stiffness k_1 and k_2 , each having a rest length ℓ_0 (see
 222 figure 1 for a sketch). The strain definition of Green-Lagrange is used, in
 223 order to account for large displacements, and the corresponding stress that
 224 is derived differs from the classical “ $F = -ku$ ” law of springs. This model
 225 is representative of thin shells under large displacements, with geometrically
 226 induced nonlinearities. More details about the model are found in Arquier
 227 et al. [24].

Denoting $u_i = x_i/\ell_0$ the displacement of the mass in the plane, the i -th spring Green-Lagrange strain reads²:

$$e_i = \frac{1}{2} \frac{\ell_i^2 - \ell_0^2}{\ell_0^2} = u_i + \frac{1}{2}(u_1^2 + u_2^2) \quad (9)$$

From now on, the values $\ell_0 = 1$ and $m = 1$ are assumed, in a given system of units, as different values only result in a scaling of the problem.

Then, the equation of motion for the mass in direction x_i reads:

$$mu_i'' + N_i + u_i(N_1 + N_2) = 0 \quad (10)$$

where $N_i = k_i e_i$ is the stress in each spring.

The system's equations of motion then reads:

$$u_i'' = -N_i - u_i(N_1 + N_2). \quad (11)$$

3.2. Continuation parameter

When calculating a family of periodic solutions of such a system using numerical continuation, a crucial problem arises: no explicit parameter exists in the system equations (10). However, as Sepulchre and MacKay [25] showed, such conservative Hamiltonian systems do have periodic orbits belonging to 1D family whose implicit parameter is the total mechanical energy of the system (the first integral). Muñoz Almaraz et al. [26] proposed to add a small dissipative term to the equation proportional to, say, λ : a parameter that will vanish along the locus of periodic solutions.

Here, the resulting dissipative, perturbed system reads:

$$u_i'' = -N_i - u_i(N_1 + N_2) - \lambda u_i' \quad i = 1, 2 \quad (12)$$

²Note that if the displacements were small, this definition could be linearized and would lead to the classical definition of the strain for a spring: $(\ell - \ell_0)/\ell_0$.

241 where λ is an explicit continuation parameter. This new system will have
 242 exactly the same periodic solutions as the original system if and only if
 243 $\lambda = 0$. Thus the standard continuation framework $\mathbf{R}(\mathbf{U}, \lambda) = 0$ can be used
 244 to compute the family of periodic solutions of this system.

245 3.3. First-order, quadratic form

Using additional variables, one can rewrite the system (12) as a set of quadratic first-order ordinary differential equations and algebraic equations as follows:

$$u'_1 = v_1 \tag{13a}$$

$$u'_2 = v_2 \tag{13b}$$

$$v'_1 = -\lambda u'_1 - N_1 - u_1(N_1 + N_2) \tag{13c}$$

$$v'_2 = -\lambda u'_2 - N_2 - u_2(N_1 + N_2) \tag{13d}$$

$$0 = N_1 - k_1 u_1 - \frac{1}{2} k_1 (u_1^2 + u_2^2) \tag{13e}$$

$$0 = N_2 - k_2 u_2 - \frac{1}{2} k_2 (u_1^2 + u_2^2) \tag{13f}$$

where (v_1, v_2) are the horizontal and vertical components of the mass velocity. The system thus has two degrees of freedom, which usually leads to only 4 state variables. However, because of the additional variables N_1 and N_2 , the (augmented) state vector has size $n = 6$:

$$\mathbf{Y}(t) = [u_1(t), u_2(t), v_1(t), v_2(t), N_1(t), N_2(t)]^t.$$

246 In what follows, the following numerical values are used: $k_1 = 1$ and
 247 $k_2 = 2$ (in the chosen system of units).

248 3.4. Convergence study

249 The first family of periodic orbits is considered, that is locally tangent
 250 (at low amplitudes) to the first oscillator linear mode: $u''_1 = -u_1$, $u_2 = 0$.

251 This family, or nonlinear normal mode, is implicitly parametrized by the
 252 total mechanical energy $E_m = \frac{1}{2}(m(v_1^2 + v_2^2) + k_1 e_1^2 + k_2 e_2^2)$. On this mode,
 253 the solution characterized by $E_m = 0.5$ is retained. To this end, a branch
 254 is computed for each discretization, and this solution point is located on the
 255 branch using a dichotomy algorithm up to a relative precision of $\epsilon_{Em} = 10^{-12}$
 256 on the total mechanical energy.

257 To assess the convergence, the relative error (in the norm 2) between each
 258 of the solutions obtained with a given approximation (i.e. the solution with
 259 a given H value in the case of the HBM, and a given N value in the case of
 260 the collocation) and a reference solution is computed. This error is evaluated
 261 in the time domain by computing the time series of the solutions sampled at
 262 2000 equidistant points over one period.

263 Denoting $\mathbf{Y}(t_i)$ the time series of the state vector of a given approximated
 264 solution (where $t_i = iT/2000$, $i=1..2000$) and $\mathbf{Y}_{\text{ref}}(t_i)$ that of the reference
 265 solution, the chosen norm reads:

$$\epsilon_r = \frac{\|[\mathbf{Y}(t_i) - \mathbf{Y}_{\text{ref}}(t_i)]_{i=1..2000}\|_2}{\|[\mathbf{Y}_{\text{ref}}(t_i)]_{i=1..2000}\|_2} \quad (14)$$

266 In the present case, the system being perfectly smooth and weakly non-
 267 linear, the Fourier series of any solution converges quickly, and the reference
 268 solution has been computed using HBM with $H = 128$ harmonics for which
 269 a very small residue norm has been achieved³: $\|\mathbf{R}(\mathbf{U}_{\text{ref}})\| = 2.95 \times 10^{-16}$.

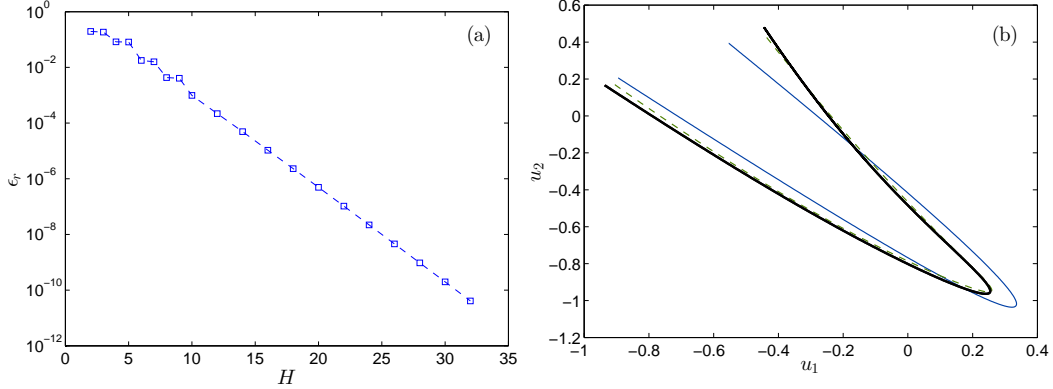


Figure 2: Convergence of HBM solutions for the weakly nonlinear system (13). The chosen solution, on each branch of periodic solutions has a total mechanical energy $E_m = 0.5$. **(a)** The norm-2 relative error ϵ_r as a function of the number of harmonics H , in semi-logarithmic scale. **(b)** Trajectories in the (u_1, u_2) plane, of the approximated solutions with $H=2$ (—, blue), 4 (—, green), 6 (— · —, red), and 8 (···, orange) as well as the reference solution (—, black). The last three trajectories are superimposed, illustrating the fast convergence.

270 3.4.1. Frequency domain approach: high-order harmonic balance

271 Figure 2 displays, in the left part (a), the evolution of the relative error ϵ_r
 272 of the approximation as a function of the number of harmonics H , in a semi-
 273 logarithmic scale. It shows the typical exponential convergence of spectral
 274 methods. The stairs-like shape of the curve at low H values suggests that odd
 275 harmonics have little influence on the error, which is explained by the fact
 276 that the chosen solution is of moderate amplitude, therefore the dominant
 277 nonlinearity of the system is quadratic.

278 The right part of figure 2 shows trajectories of several approximations as

³The authors have also confronted this reference solution by comparing it to the result of a time marching scheme that provides error control along the trajectory. Using an extremely fine tolerance criteria and starting from identical initial conditions (up to machine precision), both solutions are found to be almost identical, with a relative norm-2 difference of the order of 1×10^{-11} .

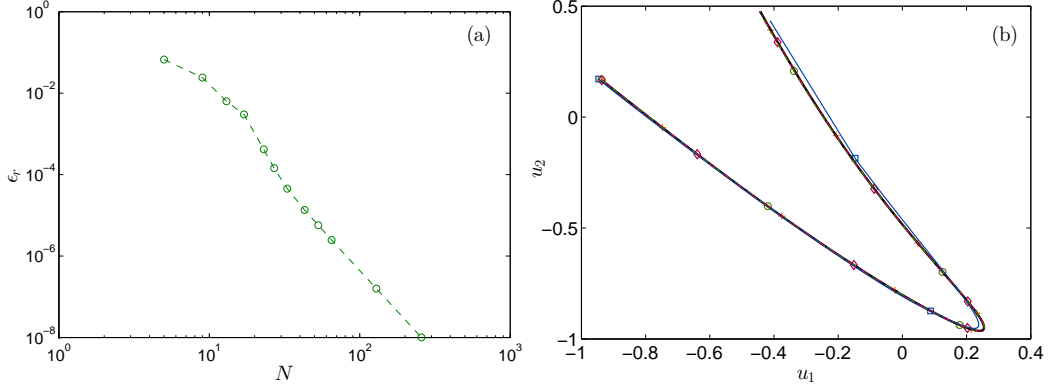


Figure 3: Convergence of orthogonal collocation with piecewise cubic polynomials on the weakly nonlinear system (13). The chosen solution, on the branch of periodic solutions has a total mechanical energy $E_m = 0.5$. **(a)** Norm-2 relative error ϵ_r as a function of the number of elements N , in logarithmic scale. **(b)** Phase diagram, in the (u_1, u_2) plane, of the approximated solutions with $N=3$ (—, squares, blue), 5 (—, circles, green), 9 (— · —, diamonds, red), and 17 (···, crosses, orange) as well as the reference solution (—, black). Markers indicate the location of the oscillator at t_j , the start of each of the N time interval subdividing the period. The last three curves are almost superimposed, illustrating the fast convergence.

279 well as of the reference solution in the (u_1, u_2) plane. The $H = 8$ solution thus
 280 is a very good approximation, both qualitatively (the trajectory is superim-
 281 posed with that of the reference solution) and quantitatively ($\epsilon_r = 4.10^{-3}$).

282 3.4.2. Time domain approach: orthogonal collocation with piecewise cubic 283 polynomials

284 Figure 3 displays, in the left part (a), the relative error of the approxi-
 285 mation ϵ_r as a function of the number of elements (logarithmic scale). In the
 286 right part (b) of that figure, the shape of several approximations as well as
 287 that of the reference solution in the (u_1, u_2) plane are shown.

288 The semi-logarithmic error-plot (not displayed) shows an exponential con-
 289 vergence for $N < 27$ (first six points from the left end), whereas the logarith-
 290 mic plot displayed here suggests an asymptotic convergence that is polyno-

291 mial in N (of order 4), for N sufficiently large. It is the expected asymptotic
 292 behavior, according to De Boor and Swartz [22], given that the system is
 293 perfectly smooth (the nonlinear terms are low order polynomials).

294 3.4.3. Comparison

295 In order to compare the two methods, the total number of equations
 296 involved in the final algebraic system needs to be taken into account. This
 297 number, denoted N_{tot} , is :

- 298 • $(2H + 1)n + 1$ in the case of the HBM,
- 299 • $(3N + 1)n + 1$ in the case of the collocation method.

300 Figure 4 clearly shows that, for this simple, smooth, weakly nonlinear
 301 system, HBM achieves a much quicker convergence. A fair comparison would
 302 require the use of a collocation with piecewise polynomials whose order p
 303 would be the refining parameter (with a fixed number of elements). However,
 304 for reasons explained above, it is beyond the scope of this study.

305 3.5. Computing a branch of periodic solutions

306 Figure 5 illustrates the branch of periodic solutions computed using HBM
 307 discretization ($H=128$ harmonics) and the ANM continuation. The mechan-
 308 ical energy along the horizontal direction $E_{m,1}=\frac{1}{2}mv_1^2 + \frac{1}{2}k_1e_1^2$ and that along
 309 the vertical direction $E_{m,2}=\frac{1}{2}mv_2^2 + \frac{1}{2}k_2e_2^2$ are plotted against the angular
 310 frequency ω . At low amplitudes (bottom-right corner), the nonlinear mode
 311 is tangent to the linear mode $(1, 0)$.

312 Figure 6 illustrates the same branch in a classical frequency-energy plot.
 313 The branch obtained using HBM ($H=128$ harmonics) and that from colloca-
 314 tion ($N=85$ elements, $p=3$ collocation points per element) are both plotted
 315 but are superimposed. Using the HBM with $H=128$ harmonics, the size

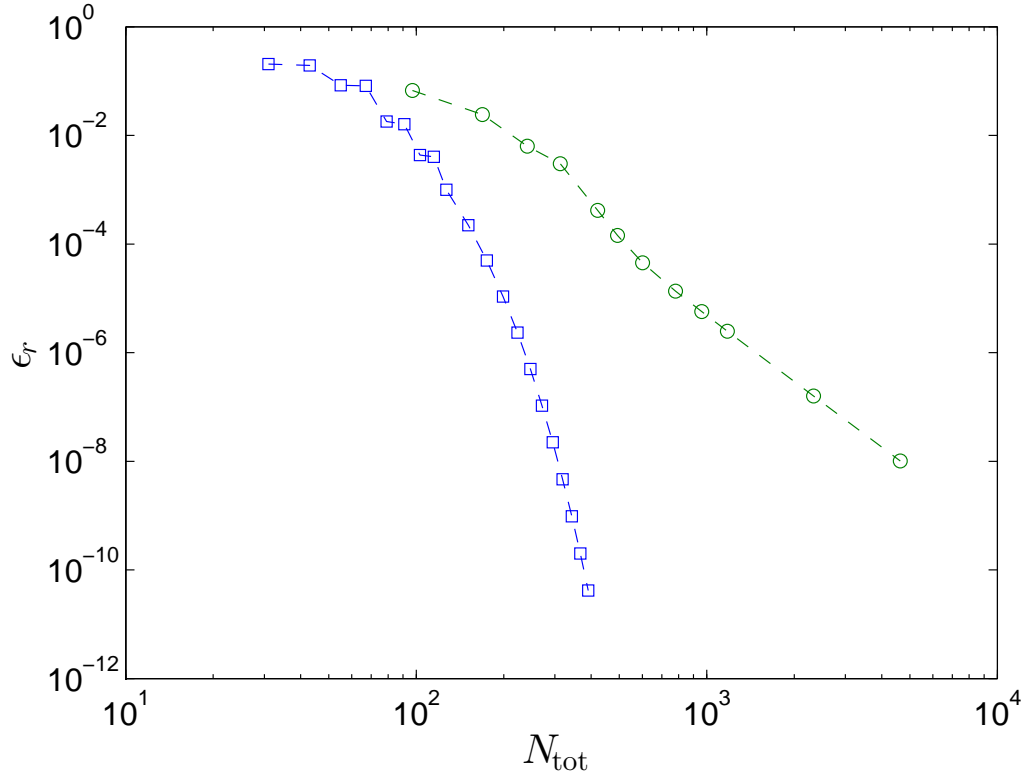


Figure 4: Norm-2 relative error (with respect to the reference solution) as a function of the total number of algebraic equations after discretization: comparison between HBM (squares, blue) and piecewise cubic polynomial collocation (circles, green).

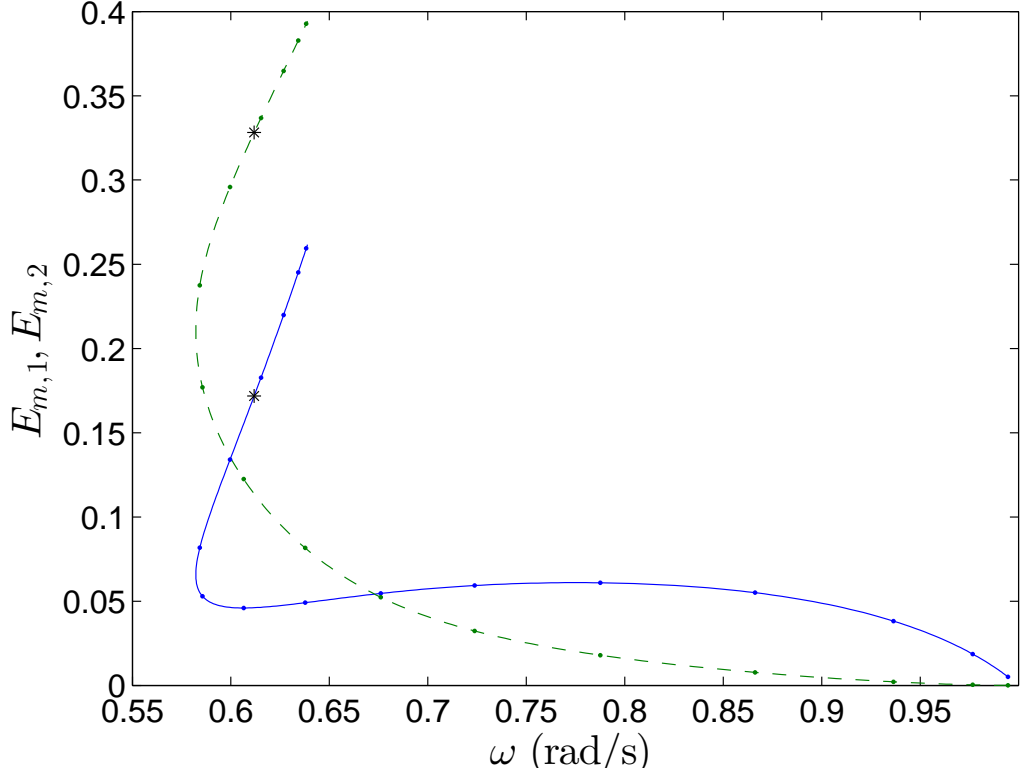


Figure 5: Branch of periodic solutions for the weakly nonlinear system (13) using HBM discretization and ANM continuation: mechanical energy of the system projected on the horizontal axis $E_{m,1}$ (—, blue) and on the vertical axis $E_{m,2}$ (---, green) as functions of the angular frequency ω . Small dots indicate the continuation steps. The black star on each curve indicates the position of the solution used for the convergence study. Reference diagram computed using $H = 128$ harmonics.

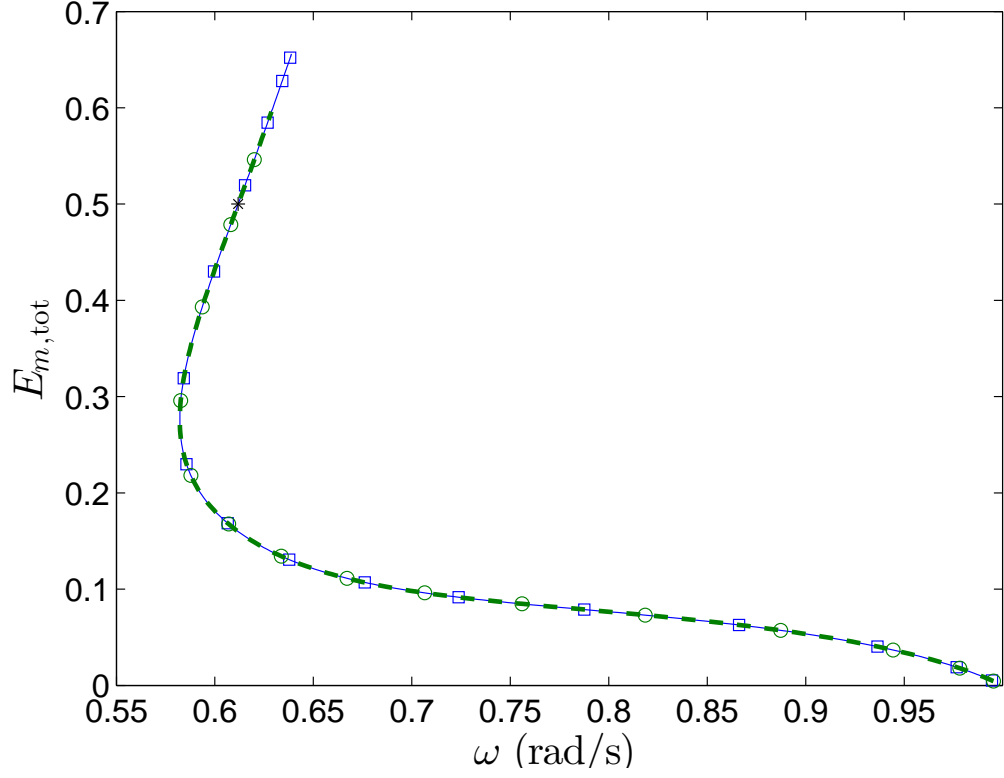


Figure 6: Branch of periodic solutions for the weakly nonlinear system (13): frequency-energy plot of the system obtained with HBM, $H=128$ harmonics (—, squares, blue) and collocation, $N=85$ cubic elements (—, circles, green). The curves are superimposed. Blue squares indicate the continuation steps of the HBM branch, while green circles indicate that of the collocation branch. The black star indicates the position of the solution used for the convergence study.

of $\mathbf{R}(\mathbf{U})$ is $N_{\text{tot}}=1543$, and the target point where $E_m=0.5$ is reached after 12 continuation steps, starting from $u_1(0)=-0.1$ and $\omega=0.995\text{rad/s}$. Using collocation with $N=85$ elements of order $p=3$, the resulting algebraic system size is $N_{\text{tot}}=1537$, and the target point with $E_m=0.5$ is reached after 14 continuation steps, from the same starting point.

To conclude the study of this weakly nonlinear system, HBM and collocation both appear to be efficient methods for computing the branch of periodic solutions with a numerical continuation tool. The HBM was found to show exponential convergence, while the collocation method showed polynomial convergence (with respect to N), as expected⁴. The next section will explore how these methods adapt to a very stiff nonlinearity.

4. Comparative study, case 2: a strongly nonlinear system

The same procedure is now applied to test both discretization methods on a stiff nonlinearity: an exponential function.

4.1. A simple oscillator impacting a rigid wall

This example consists in a one degree-of-freedom mass-spring like system, whose position is constrained in the half-plane $u < 1$ by a perfectly rigid wall, where $u(t)$ denotes the dimensionless position of the (unit) mass.

The wall reaction is regularized using an exponential function, with a coefficient α allowing for the tuning of the regularization stiffness:

$$F_r(u) = -e^{\alpha(u-1)},$$

⁴Note that increasing the order p of the polynomials instead of the number of elements N would result in an exponential convergence as for the HBM.

336 The regularized impacting oscillator is governed by the following equation
 337 of motion:

$$u''(t) = -u(t) - e^{\alpha(u(t)-1)}, \quad (15)$$

338 where the prime sign denotes time differentiation. Note that due to the form
 339 chosen for the wall reaction $F_r(u)$, the problem (15) is conservative. In what
 340 follows, the value $\alpha = 200$ is used, which corresponds to an extremely stiff
 341 regularization.

342 4.2. Continuation parameter

343 As for the first system, a dissipative perturbation is added to the system
 344 so that an explicit parameter λ appears in the equations, in order to use
 345 the classical framework $R(U, \lambda)$ for the continuation. The resulting system
 346 is now dissipative :

$$u''(t) = -u(t) - \lambda u'(t) - e^{\alpha(u(t)-1)}, \quad (16)$$

347 where λ is the continuation parameter.

348 The perturbed system (16) has exactly the same periodic solutions as
 349 that of the conservative system (15) if and only if $\lambda = 0$.

For the treatment of the exponential nonlinearity in the quadratic frame-
 work of the ANM, the reader is referred to Karkar et al. [2] and Karkar [27].
 The system is rewritten as follows:

$$u'(t) = v(t) \quad (17a)$$

$$v'(t) = -u(t) - \lambda v(t) - e(t) \quad (17b)$$

$$e'(t) = \alpha e(t)v(t) \quad (17c)$$

$$e(0) = e^{\alpha(u(0)-1)} \quad (17d)$$

Thus, the number of ordinary differential equations is $n = 3$ (the last equation is only an initial condition and does not require any discretization), with the following state vector: $Y(t) = [u(t), v(t), e(t)]^t$.

4.3. Convergence study

The periodic solution corresponding to a total mechanical energy $E_m = \frac{1}{2}(1.5)^2 = 1.125$ is retained, ie. that with maximum amplitude reached during free flight of $\|u\|_{max} = 1.5$.

Given the stiffness of the nonlinearity, one needs to ensure that both methods converge to the “right” solution. Thus, a reference solution should be either analytically computed or numerically obtained through time integration with very coarse tolerance criteria.

4.3.1. Reference solution

Because the system is very stiff, one can expect the HBM to achieve much slower convergence than in the previous case. In the worst case, the convergence may not even be uniform. Thus, for this second example, an independent method, which allows error control, was chosen to construct a reference solution.

A time marching scheme especially designed for stiff systems is used. It is a single-step solver with adaptive step size, based on a modified Rosenbrock formula of order 2 (see [28]). On each component, the relative tolerance is set to 10^{-10} and the absolute tolerance to 10^{-12} .

The reference solution is computed from the starting point $(u, v) = (-1.5, 0)$, on a time interval long enough to get more than one period. The length of the period is then deduced by analysis of the computed orbit: an event is triggered when the orbit passes over the starting point and the instant of this event is recorded.

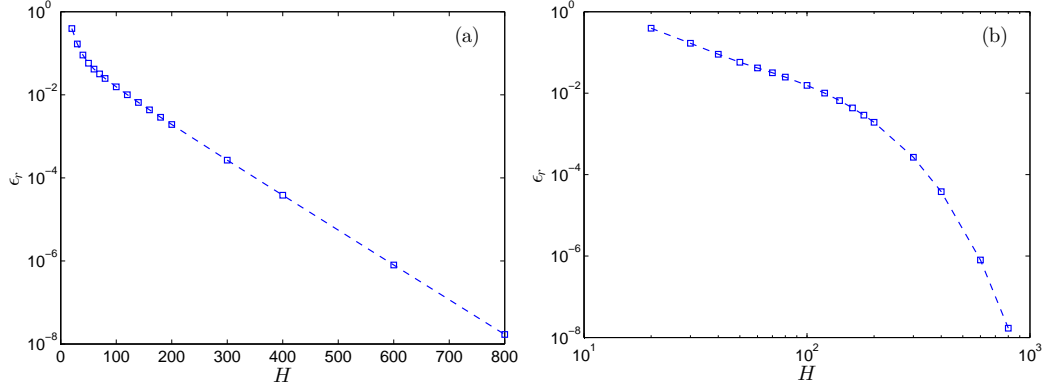


Figure 7: Convergence of the HBM for the strongly nonlinear system (17): a free, conservative impact oscillator regularized with a stiff ($\alpha=200$) exponential. Norm-2 relative error ϵ_r with respect to the reference solution, as a function of the number of harmonics H retained in the approximation. **(a)** Semi-logarithmic scale. **(b)** Logarithmic scale. The solution is such that $\|u\|_{max}=1.5$.

4.3.2. Frequency domain approach : harmonic balance method

Figure 7 illustrates convergence of the HBM. The relative error ϵ_r with respect to the reference solution is plotted against the number of harmonics H retained in the approximation.

For each H value, the branch was followed by continuation until a sufficient amplitude was reached. Then, the solution point whose amplitude is such that $\|u\|_{max}=1.5$ was extracted from the branch by a dichotomy algorithm, with a relative precision of 1.10^{-12} .

For each value of H , a time series $[\mathbf{Y}(t_i)]$ was computed that consists in 2000 equally spaced samples over one period ($t_i = iT/2000$, $i = 1..2000$) and was compared to that of the reference solution $[\mathbf{Y}_{ref}(t_i)]$ by means of the relative error ϵ_r , as defined in the previous section (see equation (14)).

The convergence plot displayed figure 7, where ϵ_r is plotted against H , shows two distinct parts:

- first, for $H < 50$ (first four points), a polynomial convergence is ob-

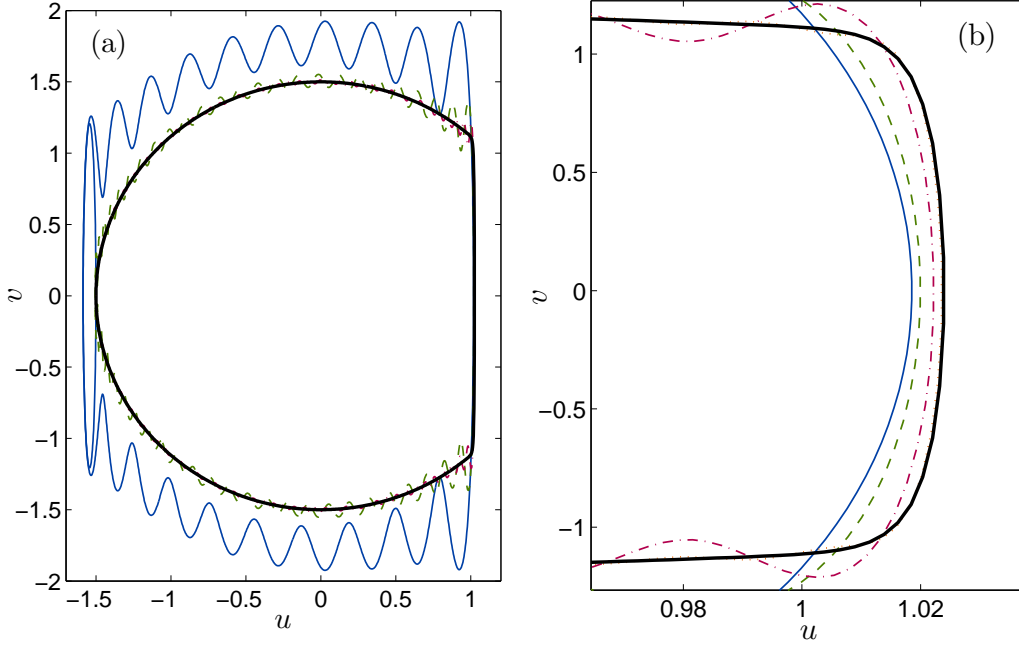


Figure 8: Phase diagram of the approximated solutions with $H=20$ (—, blue), 50 (– –, green), 100 (– · –, red), 200 (····, orange), as well as the reference solution (—, black). **(a)**: full scale diagram (the orange curve is not visible). **(b)**: zoom onto the impact zone ($u=1$), where all curves can be distinguished (orange and black almost superimposed).

served (straight line on a logarithmic scale), probably due to the fact that the approximation with such a low H value is not able to capture the sudden variations of trajectory during the impact;

- then, for $H > 50$, an exponential convergence is obtained (straight line on a semi-logarithmic scale), which is the expected asymptotic convergence of the HBM applied to a smooth system.

The phase diagram plotted on figure 8 is a perfect illustration of the observed phenomenon in the first convergence regime: the approximation is very crude with $H=20$, but tends quickly to the reference solution as H is increased, at least at the scale of the entire orbit. Refining the approximation with more than 100 harmonics only produces visible effects close to the stiff

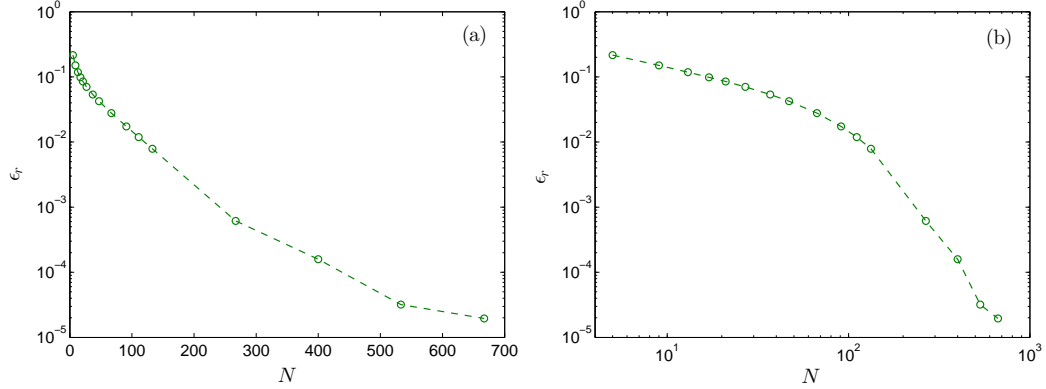


Figure 9: Convergence study of the collocation method for the strongly nonlinear system (17): a free, conservative impact oscillator regularized with a stiff ($\alpha=200$) exponential. Chosen cycle amplitude: $\|u\|_{max}=1.5$. Norm-2, relative error with respect to a reference solution as a function of the number of elements N . **(a)** Semilogarithmic scale. **(b)** Logarithmic scale.

part of the orbit, near $u=1$, where the approximation with $H = 200$ can actually be distinguished from the reference solution. A slight penetration (approximately 2% of the total amplitude of the cycle) inside the “wall” is observed, as a result of the regularization. By tuning the α parameter, one can control this penetration, with respect to the cycle amplitude⁵.

4.3.3. Time domain approach: orthogonal collocation with piecewise polynomials

The same analyses are now applied to the collocation method. The relative error is computed using the same definition as in the previous parts. Values of (u, v) at t_i are interpolated using cubic polynomials⁶.

Figure 9 illustrates how the collocation method converges in three parts:

⁵One could also finely tune both the penetration and the stiffness of the system by using an additional multiplicative parameter in front of the exponential term.

⁶By definition, the elements used are cubic polynomials, written in the Lagrange basis defined on four equally spaced points, including borders. See section 2.

- 413 • first for $N \leq 27$, the relative error decreases polynomially (low order)
414 in N : the first six points on the right plot (b), with a logarithmic scale,
415 form a straight line;
- 416 • then for $27 \leq N \leq 267$, the convergence seems exponential in N : the
417 corresponding points on the left plot (a), with a semi-logarithmic scale,
418 form a straight line;
- 419 • finally for $N \geq 267$, the convergence seems polynomial (high order) in
420 N .

421 In the last part of the figure, the points being not perfectly aligned suggest
422 the asymptotic behavior is not yet reached.

423 In the case of a very smooth problem, Karniadakis and Sherwin [20]
424 showed that it is more efficient to use higher degree interpolants than increas-
425 ing the number of elements N . However, the “smoothness” of the problem
426 is resolved after a minimal number of elements. Put differently, the stiffness
427 of the system makes the transition (before reaching asymptotic convergence
428 rates) longer. The low-order (~ 1) polynomial convergence is the result of
429 the stiffness of the solution, and increasing the degree of the interpolants
430 would probably not make the error decrease faster.

431 Thus, in the present case, increasing N is probably more efficient, at least
432 up to $N=267$. Only after this point, where the high-order (~ 3) polynomial
433 convergence is observed, may a p -refinement be preferable (for extremely high
434 accuracy computations).

435 Figure 10 illustrates the phase diagram (u, v) of several approximations
436 of the solution. Element boundaries are plotted using markers. Until $N=67$,
437 one observes that the number of elements is too low to have at least one
438 element inside the stiff part of the orbit (impact). For higher values of N ,

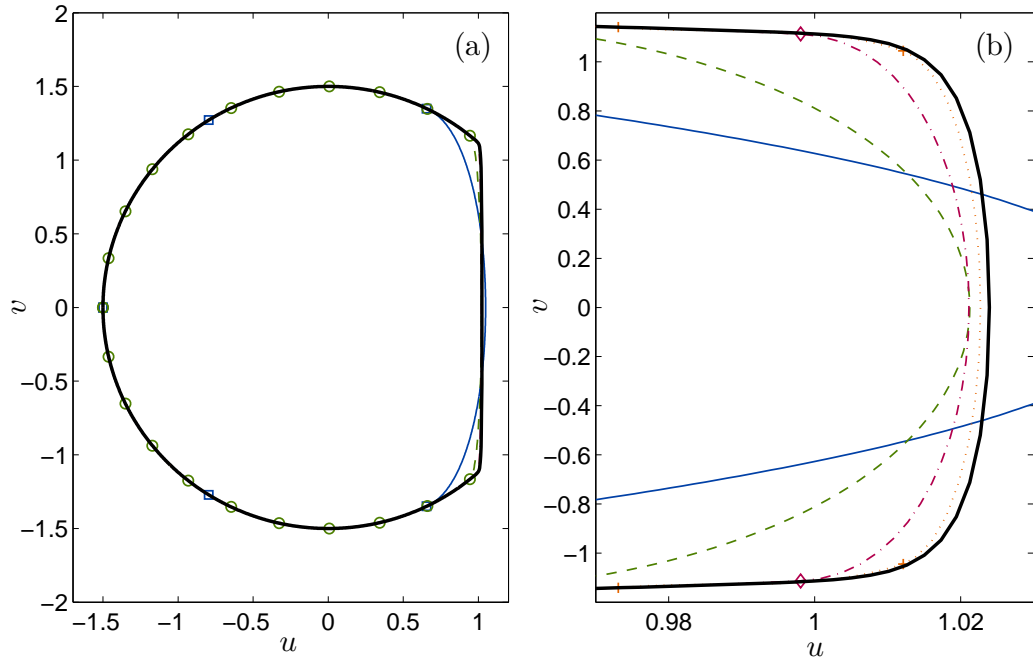


Figure 10: Phase diagram of approximated solutions using $N=5$ (—, squares, blue), 21 (---, circles, green), 67 (- · -, diamonds, red), and 133 (···, crosses, orange) as well as the reference solution (—, black). **(a)** Full scale; markers show the element boundaries for the first two approximations (5 and 21 elements respectively). **(b)** Zoom onto the impact zone ($u=1$); markers (diamonds and crosses) indicate the element boundaries for approximations corresponding to 67 and 133 elements.

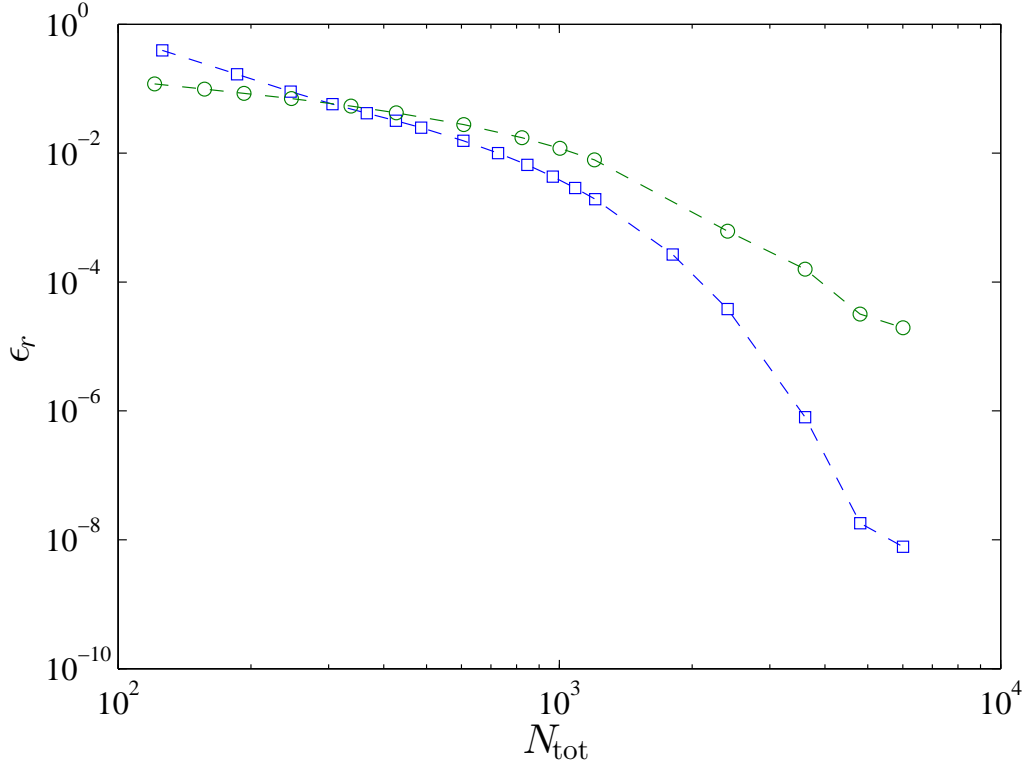


Figure 11: Comparison between harmonic balance (squares, blue) and collocation (circles, green): norm-2 relative error with respect to a reference solution as a function of the size of the final algebraic system (resulting from discretization). Case of the impacting oscillator regularized with a stiff exponential ($\alpha=200$). Solution amplitude for the comparison: $\|u\|_{max}=1.5$.

439 element boundaries penetrate inside the stiff part of the orbit, allowing for a
 440 better representation of the solution as derivative discontinuities are possible
 441 at these points.

442 4.3.4. Comparison

443 Figure 11 shows the comparison of convergence curves for the two meth-
 444 ods: $\epsilon_r=f(N_{\text{tot}})$, where the abscissa is the total size of the algebraic system
 445 resulting from the discretization:

- 446 • $N_{\text{tot}} = (2H + 1)n + 3$ for the HBM⁷,
- 447 • and $N_{\text{tot}} = (3N + 1)n + 1$ for the collocation method.

448 Even though the approximation of the solution using a Fourier series
 449 with relatively few harmonics ($H < 50$) is relatively poor, the convergence
 450 rate gives the HBM an advantage. While the tangent matrix resulting from
 451 harmonic balance is less sparse and has a much greater bandwidth than that
 452 of a collocation method (thus, the computation time needed to compute
 453 this matrix and to invert it is longer, especially for very high H values), the
 454 convergence shows that for a given accuracy, a much smaller system is needed
 455 with the HBM than with the collocation.

456 Finally, given the limited resources of a classical PC workstation, the
 457 HBM allows for the computation of a much more precise solution compared
 458 to the collocation.

459 4.4. Continuation of periodic solutions

460 The branches of periodic solutions computed using both discretization
 461 techniques are shown in figure 12. Using ANM series up to order 20, and
 462 starting from the linear solution at $\|u\|_{\text{max}}=0.9$, it takes 26 steps to reach the
 463 point that corresponds to the solution ($\|u\|_{\text{max}}=1.5$) when using the HBM,
 464 while it takes 36 steps with the collocation method. The computation was
 465 carried out, in the first case, with $H=1000$ harmonics ($N_{\text{tot}}=6006$) and in
 466 the second case with $N=667$ ($N_{\text{tot}}=6007$). Both methods show a shortening
 467 of steps around the linear-nonlinear transition (expected result). However,
 468 the HBM leads to larger steps further down the branch, while the collocation
 469 leads to more or less constant (or even decreasing) step sizes.

⁷Note that there are two more variables than for the previous test case, because of additional variables $e(0)$ and $u(0)$ needed for the definition of initial condition 17d.

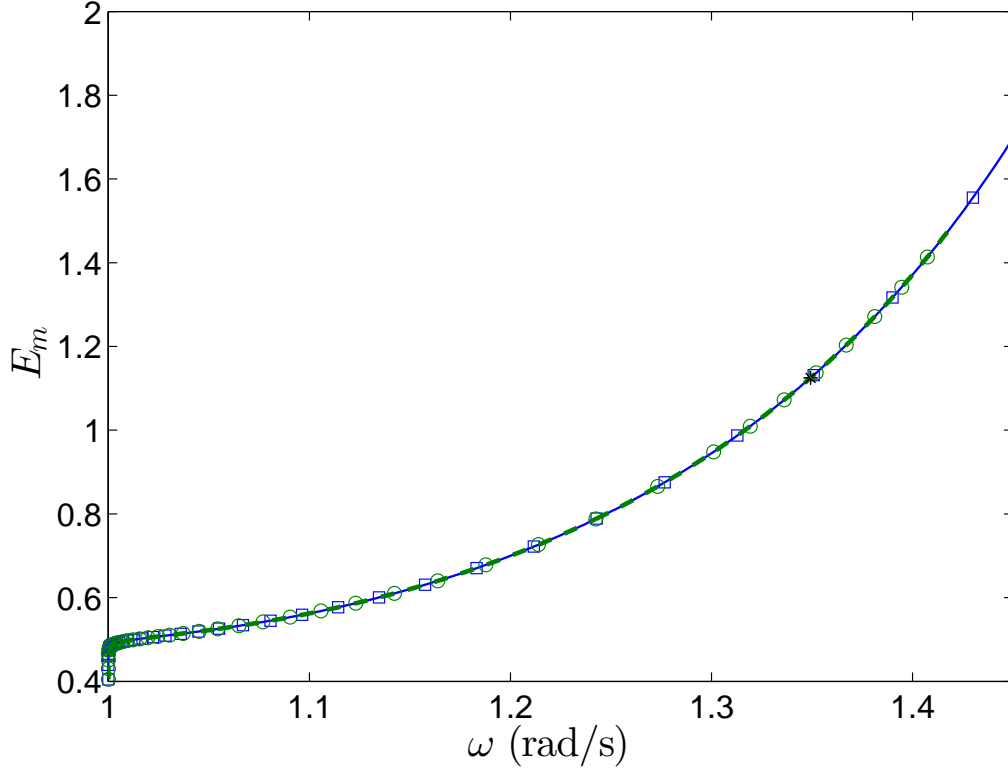


Figure 12: Frequency-energy plot of the branch of periodic solutions computed using HBM (—, squares, blue) and collocation (—, circles, green) for the regularized impacting oscillator. Markers indicate the beginning of each continuation step. The star denotes the solution used in the convergence study. Fourier series order for the HBM: $H=1000$. Number of cubic elements for the collocation: $N=667$. Regularization parameter: $\alpha=200$. All parameters of the ANM are identical to the previous example.

470 5. Conclusion

471 Two discretization methods for solving periodic boundary value problems
472 were compared: the harmonic balance, which is based on the frequency do-
473 main, and the orthogonal collocation (at Gauss points) with piecewise poly-
474 nomials, which is based on the time domain. The methods were compared
475 to each other in terms of convergence, and as means to compute branch of
476 periodic solutions using numerical continuation.

477 The main conclusion is that, in the absence of basis enrichment or adap-
478 tive harmonic selection (for the HBM), and without adaptive mesh or p-
479 refinement (for the collocation), the harmonic balance method achieves bet-
480 ter convergence rates, and thus allows for much more precise approximations,
481 even in the case of very stiff systems. This is surprising since the spectrum
482 is expected to be greatly enlarged by a stiff nonlinearity, and a time-based
483 method could seem more appropriate to discretize such stiff solutions.

484 Of course, improvements exist for both methods. On the one hand, col-
485 location methods have proved to be more efficient when using an adaptive
486 mesh (the AUTO software [16] is a well known implementation). On the other
487 hand, adaptive harmonic selection and basis enrichment are also known to
488 improve drastically the convergence of the harmonic balance for non-smooth
489 problems (see e.g. Kim and Perkins [12])

490 The lack of comparison in the literature is to be underlined, possibly due
491 to the difficulty to apply the HBM at very high orders (here, up to 1000
492 harmonics) until recently. Further comparison using improved methods are
493 needed.

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